GEOMETRY OF AN ISOLATED DIMER OF IMIDAZOLE CHARACTERISED BY ROTATIONAL SPECTROSCOPY AND AB INITIO CALCULATIONS

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An isolated, gas-phase dimer of imidazole is generated through laser vaporisation of a solid rod containing a 1:1 mixture of imidazole and copper in the presence of an argon buffer gas undergoing supersonic expansion. The complex is characterised through broadband rotational spectroscopy and is shown to have a twisted, hydrogen-bonded geometry. Calculations at the CCSD(T)(F12*)/cc-pVDZ-F12 level of theory confirm this to be the lowest-energy conformer of the imidazole dimer. The distance between the respective centres of mass of the imidazole monomer subunits is determined to be 5.2751(1) Å, and the twist angle γ describing rotation of one monomer with respect to the other about a line connecting the centres of mass of the monomers is determined to be $87.9(4)^o$. Four out of six intermolecular parameters in the model geometry are precisely determined from the experimental rotational constants and are consistent with results calculated ab initio.